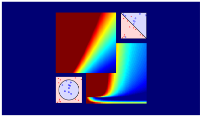
Machine Learning Foundations
(機器學習基石)



Lecture 14: Regularization

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Roadmap

1. When Can Machines Learn?
2. Why Can Machines Learn?
3. How Can Machines Learn?
4. How Can Machines Learn **Better**?

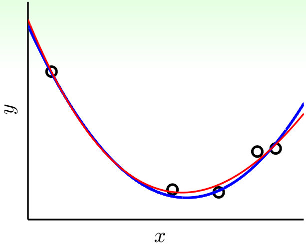
Lecture 13: Hazard of Overfitting

overfitting happens with **excessive power**, **stochastic/deterministic noise**, and **limited data**

Lecture 14: Regularization

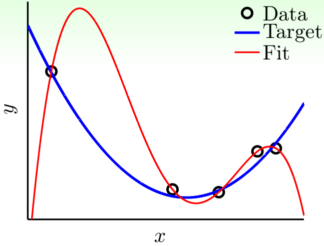
- Regularized Hypothesis Set
- Weight Decay Regularization
- Regularization and VC Theory
- General Regularizers

Regularization: The Magic



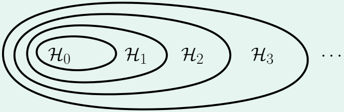
'regularized fit'

$\Longleftarrow$



overfit

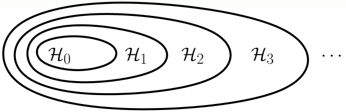
- idea: 'step back' from $\mathcal{H}_{10}$ to $\mathcal{H}_2$



- name history: function approximation for **ill-posed problems**

how to step back?

Stepping Back as Constraint



Q-th order polynomial transform for $x \in \mathbb{R}$:

$$\mathbf{\Phi}_Q(x) = \left(1, x, x^2, \ldots, x^Q\right)$$

+ linear regression, denote $\tilde{\mathbf{w}}$ by $\mathbf{w}$

hypothesis **w** in $\mathcal{H}_{10}$: $w_0 + w_1 x + w_2 x^2 + w_3 x^3 + \ldots + w_{10} x^{10}$

hypothesis **w** in $\mathcal{H}_2$: $w_0 + w_1 x + w_2 x^2$

that is, $\mathcal{H}_2 = \mathcal{H}_{10}$ AND 'constraint that $w_3 = w_4 = \ldots = w_{10} = 0$'

step back = **constraint**

Regression with Constraint

$$\mathcal{H}_{10} \equiv \left\{ \mathbf{w} \in \mathbb{R}^{10+1} \right\}$$

regression with $\mathcal{H}_{10}$:

$$\min_{\mathbf{w} \in \mathbb{R}^{10+1}} E_{\text{in}}(\mathbf{w})$$

$$\mathcal{H}_2 \equiv \left\{ \mathbf{w} \in \mathbb{R}^{10+1} \text{ while } w_3 = w_4 = \ldots = w_{10} = 0 \right\}$$

regression with $\mathcal{H}_2$:

$$\min_{\mathbf{w} \in \mathbb{R}^{10+1}} E_{\text{in}}(\mathbf{w}) \quad \text{s.t.} \quad w_3 = w_4 = \ldots = w_{10} = 0$$

step back = constrained optimization of E_{in}

why don't you just use $\mathbf{w} \in \mathbb{R}^{2+1}$? **:-)**

Regression with Looser Constraint

$\mathcal{H}_2 \equiv \Big\{ \mathbf{w} \in \mathbb{R}^{10+1}$ while $w_3 = \ldots = w_{10} = 0 \Big\}$

regression with $\mathcal{H}_2$:

$$\min_{\mathbf{w} \in \mathbb{R}^{10+1}} E_{\text{in}}(\mathbf{w}) \quad \text{s.t.} \quad w_3 = \ldots = w_{10} = 0$$

$\mathcal{H}'_2 \equiv \Big\{ \mathbf{w} \in \mathbb{R}^{10+1}$ while ≥ 8 of $w_q = 0 \Big\}$

regression with $\mathcal{H}'_2$:

$$\min_{\mathbf{w} \in \mathbb{R}^{10+1}} E_{\text{in}}(\mathbf{w}) \quad \text{s.t.} \quad \sum_{q=0}^{10} [\![w_q \neq 0]\!] \leq 3$$

- more flexible than $\mathcal{H}_2$: $\mathcal{H}_2 \subset \mathcal{H}'_2$
- less risky than $\mathcal{H}_{10}$: $\mathcal{H}'_2 \subset \mathcal{H}_{10}$

bad news for sparse hypothesis set $\mathcal{H}'_2$:
NP-hard to solve :-(

Regression with Softer Constraint

$$\mathcal{H}_2' \equiv \left\{ \mathbf{w} \in \mathbb{R}^{10+1} \text{ while } \geq 8 \text{ of } w_q = 0 \right\}$$

regression with $\mathcal{H}_2'$:

$$\min_{\mathbf{w} \in \mathbb{R}^{10+1}} E_{\text{in}}(\mathbf{w}) \text{ s.t. } \sum_{q=0}^{10} [\![w_q \neq 0]\!] \leq 3$$

$$\mathcal{H}(C) \equiv \left\{ \mathbf{w} \in \mathbb{R}^{10+1} \text{ while } \|\mathbf{w}\|^2 \leq C \right\}$$

regression with $\mathcal{H}(C)$:

$$\min_{\mathbf{w} \in \mathbb{R}^{10+1}} E_{\text{in}}(\mathbf{w}) \text{ s.t. } \sum_{q=0}^{10} w_q^2 \leq C$$

- $\mathcal{H}(C)$: overlaps but not exactly the same as $\mathcal{H}_2'$
- soft and smooth structure over $C \geq 0$:
  $\mathcal{H}(0) \subset \mathcal{H}(1.126) \subset \ldots \subset \mathcal{H}(1126) \subset \ldots \subset \mathcal{H}(\infty) = \mathcal{H}_{10}$

regularized hypothesis $\mathbf{w}_{\text{REG}}$:
optimal solution from
regularized hypothesis set $\mathcal{H}(C)$

Fun Time

For $Q \geq 1$, which of the following hypothesis (weight vector $\mathbf{w} \in \mathbb{R}^{Q+1}$) is not in the regularized hypothesis set $\mathcal{H}(1)$?

1. $\mathbf{w}^T = [0, 0, \ldots, 0]$
2. $\mathbf{w}^T = [1, 0, \ldots, 0]$
3. $\mathbf{w}^T = [1, 1, \ldots, 1]$
4. $\mathbf{w}^T = \left[\sqrt{\frac{1}{Q+1}}, \sqrt{\frac{1}{Q+1}}, \ldots, \sqrt{\frac{1}{Q+1}}\,\right]$

Fun Time

For $Q \geq 1$, which of the following hypothesis (weight vector $\mathbf{w} \in \mathbb{R}^{Q+1}$) is not in the regularized hypothesis set $\mathcal{H}(1)$?

1. $\mathbf{w}^T = [0, 0, \ldots, 0]$
2. $\mathbf{w}^T = [1, 0, \ldots, 0]$
3. $\mathbf{w}^T = [1, 1, \ldots, 1]$
4. $\mathbf{w}^T = \left[\sqrt{\frac{1}{Q+1}}, \sqrt{\frac{1}{Q+1}}, \ldots, \sqrt{\frac{1}{Q+1}}\right]$

Reference Answer: ③

The squared length of $\mathbf{w}$ in ③ is $Q + 1$, which is not ≤ 1.

Matrix Form of Regularized Regression Problem

$$\min_{\mathbf{w}\in\mathbb{R}^{Q+1}} \quad E_{\text{in}}(\mathbf{w}) = \frac{1}{N}\underbrace{\sum_{n=1}^{N}(\mathbf{w}^T\mathbf{z}_n - y_n)^2}_{(\mathrm{Z}\mathbf{w}-\mathbf{y})^T(\mathrm{Z}\mathbf{w}-\mathbf{y})}$$

$$\text{s.t.} \quad \underbrace{\sum_{q=0}^{Q} w_q^2}_{\mathbf{w}^T\mathbf{w}} \le C$$

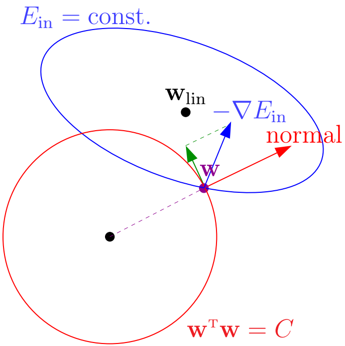
- $\sum_n \ldots = (\mathrm{Z}\mathbf{w} - \mathbf{y})^T(\mathrm{Z}\mathbf{w} - \mathbf{y})$, **remember? :-)**
- $\mathbf{w}^T\mathbf{w} \le C$: feasible $\mathbf{w}$ within a radius-$\sqrt{C}$ hypersphere

how to solve
constrained optimization problem?

The Lagrange Multiplier

$$\min_{\mathbf{w}\in\mathbb{R}^{Q+1}} \quad E_{\text{in}}(\mathbf{w}) = \frac{1}{N}(\mathrm{Z}\mathbf{w}-\mathbf{y})^T(\mathrm{Z}\mathbf{w}-\mathbf{y}) \text{ s.t. } \mathbf{w}^T\mathbf{w} \le C$$

- decreasing direction: $-\nabla E_{\text{in}}(\mathbf{w})$, **remember? :-)**
- normal vector of $\mathbf{w}^T\mathbf{w} = C$: $\mathbf{w}$
- if $-\nabla E_{\text{in}}(\mathbf{w})$ and $\mathbf{w}$ not parallel: can **decrease $E_{\text{in}}(\mathbf{w})$ without violating the constraint**
- at optimal solution $\mathbf{w}_{\text{REG}}$, $-\nabla E_{\text{in}}(\mathbf{w}_{\text{REG}}) \propto \boxed{\mathbf{w}_{\text{REG}}}$



want: find Lagrange multiplier $\lambda > 0$ and $\mathbf{w}_{\text{REG}}$ such that $\nabla E_{\text{in}}(\mathbf{w}_{\text{REG}}) + \frac{2\lambda}{N}\boxed{\mathbf{w}_{\text{REG}}} = \mathbf{0}$

Augmented Error

- if oracle tells you $\lambda > 0$, then

solving $$\nabla E_{\text{in}}(\mathbf{w}_{\text{REG}}) + \frac{2\lambda}{N}\boxed{\mathbf{w}_{\text{REG}}} = \mathbf{0}$$

$$\frac{2}{N}\left(\mathrm{Z}^T\mathrm{Z}\mathbf{w}_{\text{REG}} - \mathrm{Z}^T\mathbf{y}\right) + \frac{2\lambda}{N}\boxed{\mathbf{w}_{\text{REG}}} = \mathbf{0}$$

- optimal solution:

$$\mathbf{w}_{\text{REG}} \leftarrow (\mathrm{Z}^T\mathrm{Z} + \lambda\mathrm{I})^{-1}\mathrm{Z}^T\mathbf{y}$$

—called ridge regression in Statistics

minimizing unconstrained E_{aug} effectively
minimizes some C-constrained E_{in}

Augmented Error

- if oracle tells you $\lambda > 0$, then

$$\text{solving} \quad \nabla E_{\text{in}}(\mathbf{w}_{\text{REG}}) + \frac{2\lambda}{N} \boxed{\mathbf{w}_{\text{REG}}} = \mathbf{0}$$

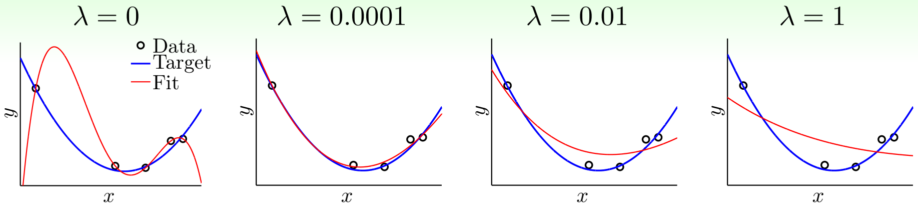
$$\text{equivalent to minimizing} \quad \underbrace{E_{\text{in}}(\mathbf{w}) + \frac{\lambda}{N} \overbrace{\mathbf{w}^T\mathbf{w}}^{\textbf{regularizer}}}_{\textbf{augmented error } E_{\text{aug}}(\mathbf{w})}$$

- regularization with augmented error instead of constrained E_{in}

$$\mathbf{w}_{\text{REG}} \leftarrow \underset{\mathbf{w}}{\text{argmin}}\, E_{\text{aug}}(\mathbf{w}) \text{ for given } \lambda > 0 \text{ or } \lambda = 0$$

minimizing unconstrained E_{aug} effectively
minimizes some C-constrained E_{in}

The Results



overfitting $\Longrightarrow$ $\Longrightarrow$ $\Longrightarrow$ underfitting

philosophy: *a little **regularization** goes a long way!*

call '$+\frac{\lambda}{N}\mathbf{w}^T\mathbf{w}$' **weight-decay** regularization:

larger λ
$\Longleftrightarrow$ prefer shorter $\mathbf{w}$
$\Longleftrightarrow$ effectively smaller C

—go with 'any' transform + linear model

Some Detail: Legendre Polynomials

$$\min_{\mathbf{w} \in \mathbb{R}^{Q+1}} \frac{1}{N} \sum_{n=0}^{N} (\mathbf{w}^T \mathbf{\Phi}(x_n) - y_n)^2 + \frac{\lambda}{N} \sum_{q=0}^{Q} w_q^2$$

naïve polynomial transform:

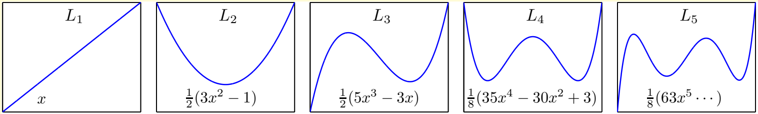
$$\mathbf{\Phi}(\mathbf{x}) = \left(1, x, x^2, \ldots, x^Q\right)$$

—when $x_n \in [-1, +1]$, x_n^q really small, needing large w_q

normalized polynomial transform:

$$\left(1, L_1(x), L_2(x), \ldots, L_Q(x)\right)$$

—'orthonormal basis functions' called Legendre polynomials



Fun Time

When would $\mathbf{w}_{\text{REG}}$ equal $\mathbf{w}_{\text{LIN}}$?

1. $\lambda = 0$
2. $C = \infty$
3. $C \geq \|\mathbf{w}_{\text{LIN}}\|^2$
4. all of the above

Fun Time

When would $\mathbf{w}_{\text{REG}}$ equal $\mathbf{w}_{\text{LIN}}$?

1. $\lambda = 0$
2. $C = \infty$
3. $C \geq \|\mathbf{w}_{\text{LIN}}\|^2$
4. all of the above

Reference Answer: (4)

(1) and (2) shall be easy; (3) means that there are effectively no constraint on **w**, hence the equivalence.

Regularization and VC Theory

Regularization by Constrained-Minimizing E_{in}

$$\min_{\mathbf{w}} E_{\text{in}}(\mathbf{w}) \text{ s.t. } \mathbf{w}^T\mathbf{w} \leq C$$

$\longrightarrow$

VC Guarantee of Constrained-Minimizing E_{in}

$$E_{\text{out}}(\mathbf{w}) \leq E_{\text{in}}(\mathbf{w}) + \Omega(\mathcal{H}(C))$$

$\Updownarrow$ C equivalent to some λ

Regularization by Minimizing E_{aug}

$$\min_{\mathbf{w}} E_{\text{aug}}(\mathbf{w}) = E_{\text{in}}(\mathbf{w}) + \frac{\lambda}{N}\mathbf{w}^T\mathbf{w}$$

minimizing E_{aug}: indirectly getting VC guarantee **without confining to** $\mathcal{H}(C)$

Another View of Augmented Error

Augmented Error

$$E_{\text{aug}}(\mathbf{w}) = E_{\text{in}}(\mathbf{w}) + \frac{\lambda}{N}\mathbf{w}^T\mathbf{w}$$

VC Bound

$$E_{\text{out}}(\mathbf{w}) \leq E_{\text{in}}(\mathbf{w}) + \Omega(\mathcal{H})$$

- regularizer $\mathbf{w}^T\mathbf{w}$: complexity of a single hypothesis
- generalization price $\Omega(\mathcal{H})$: complexity of a hypothesis set
- if $\frac{\lambda}{N}\Omega(\mathbf{w})$ 'represents' $\Omega(\mathcal{H})$ well,
  E_{aug} is a better proxy of E_{out} than E_{in}

minimizing E_{aug}:

(heuristically) operating with the better proxy;
(technically) enjoying flexibility of whole $\mathcal{H}$

Effective VC Dimension

$$\min_{\mathbf{w}\in\mathbb{R}^{\tilde{d}+1}} E_{\text{aug}}(\mathbf{w}) = E_{\text{in}}(\mathbf{w}) + \frac{\lambda}{N}\Omega(\mathbf{w})$$

- model complexity?
  $d_{\text{VC}}(\mathcal{H}) = \tilde{d} + 1$, because $\{\mathbf{w}\}$ '**all considered**' during minimization
- $\{\mathbf{w}\}$ '**actually needed**': $\mathcal{H}(C)$, with some C equivalent to λ
- $d_{\text{VC}}\big(\mathcal{H}(C)\big)$:
  effective VC dimension $d_{\text{EFF}}(\mathcal{H}, \underbrace{\mathcal{A}}_{\min E_{\text{aug}}})$

explanation of regularization:
$d_{\text{VC}}(\mathcal{H})$ large,
while $d_{\text{EFF}}(\mathcal{H}, \mathcal{A})$ small if $\mathcal{A}$ regularized

Fun Time

Consider the weight-decay regularization with regression. When increasing λ in $\mathcal{A}$, what would happen with $d_{\text{EFF}}(\mathcal{H}, \mathcal{A})$?

1. $d_{\text{EFF}} \uparrow$
2. $d_{\text{EFF}} \downarrow$
3. $d_{\text{EFF}} = d_{\text{VC}}(\mathcal{H})$ and does not depend on λ
4. $d_{\text{EFF}} = 1126$ and does not depend on λ

Fun Time

Consider the weight-decay regularization with regression. When increasing λ in $\mathcal{A}$, what would happen with $d_{\text{EFF}}(\mathcal{H}, \mathcal{A})$?

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4. $d_{\text{EFF}} = 1126$ and does not depend on λ

Reference Answer: ②

larger λ
$\Longleftrightarrow$ smaller C
$\Longleftrightarrow$ smaller $\mathcal{H}(C)$
$\Longleftrightarrow$ smaller d_{EFF}

General Regularizers $\Omega(\mathbf{w})$

want: constraint in the **'direction' of target function**

- target-dependent: some properties of target, if known
  - symmetry regularizer: $\sum [\![q \text{ is odd}]\!]\, w_q^2$
- plausible: direction towards smoother or simpler

  stochastic/deterministic noise both **non-smooth**

  - sparsity (L1) regularizer: $\sum |w_q|$ (next slide)
- friendly: easy to optimize
  - weight-decay (L2) regularizer: $\sum w_q^2$
- bad? **:-)**: no worries, guard by λ

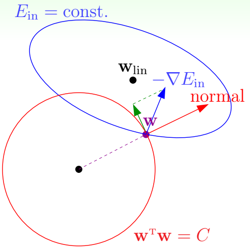
augmented error = error $\widehat{\text{err}}$ + regularizer Ω

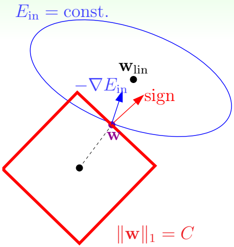
regularizer: target-dependent, plausible, or friendly

ringing a bell? :-)

error measure: user-dependent, plausible, or friendly

L2 and L1 Regularizer





L2 Regularizer

$$\Omega(\mathbf{w}) = \sum_{q=0}^{Q} w_q^2 = \|\mathbf{w}\|_2^2$$

- convex, differentiable everywhere
- easy to optimize

L1 Regularizer

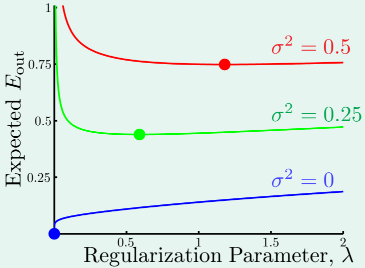
$$\Omega(\mathbf{w}) = \sum_{q=0}^{Q} |w_q| = \|\mathbf{w}\|_1$$

- convex, **not** differentiable everywhere
- **sparsity** in solution

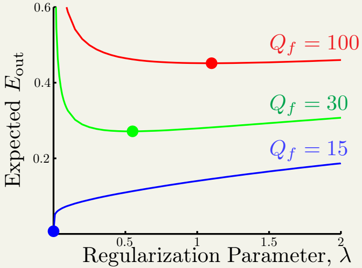
L1 useful if needing **sparse solution**

The Optimal λ

stochastic noise



deterministic noise



- more noise $\iff$ more regularization needed
  —more bumpy road $\iff$ putting brakes more
- noise **unknown**—important to **make proper choices**

how to choose?
stay tuned for the next lecture! :-)

Fun Time

Consider using a regularizer $\Omega(\mathbf{w}) = \sum_{q=0}^{Q} 2^q w_q^2$ to work with Legendre polynomial regression. Which kind of hypothesis does the regularizer prefer?

1. symmetric polynomials satisfying $h(x) = h(-x)$
2. low-dimensional polynomials
3. high-dimensional polynomials
4. no specific preference

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Consider using a regularizer $\Omega(\mathbf{w}) = \sum_{q=0}^{Q} 2^q w_q^2$ to work with Legendre polynomial regression. Which kind of hypothesis does the regularizer prefer?

1. symmetric polynomials satisfying $h(x) = h(-x)$
2. low-dimensional polynomials
3. high-dimensional polynomials
4. no specific preference

Reference Answer: ②

There is a higher 'penalty' for higher-order terms, and hence the regularizer prefers low-dimensional polynomials.

Summary

1. When Can Machines Learn?
2. Why Can Machines Learn?
3. How Can Machines Learn?
4. How Can Machines Learn **Better**?

Lecture 13: Hazard of Overfitting

Lecture 14: Regularization

- Regularized Hypothesis Set
  original $\mathcal{H}$ + constraint
- Weight Decay Regularization
  add $\frac{\lambda}{N}\mathbf{w}^T\mathbf{w}$ in E_{aug}
- Regularization and VC Theory
  regularization decreases d_{EFF}
- General Regularizers
  target-dependent, [plausible], or [friendly]

- **next: choosing from the so-many models/parameters**